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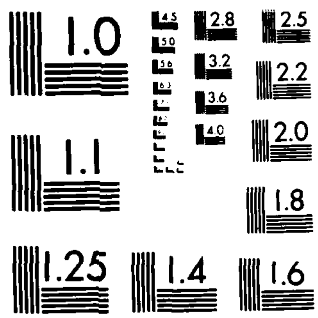
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This paper reviews methods for the parameterization of orthogonal matrices. Examples of where such parameterization can be used are presented.

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THE PARAMETERIZATION OF ORTHOGONAL MATRICES: A REVIEW MAINLY FOR STATISTICIANS

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THE PARAMETERIZATION OF ORTHOGONAL MATRICES: A REVIEW MAINLY FOR STATISTICIANS[1]

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Abstract

Techniques and applications for the parameterization of orthogonal matrices are surveyed, mainly for the benefit of statisticians.

1. Introduction.

By an orthogonal matrix $\underset{\sim}{C}$ we shall mean a real square matrix of order $n \times n$ for which $\underset{\sim}{C}\underset{\sim}{C}'$ is the identity matrix, where $\underset{\sim}{C}'$ denotes the transpose of $\underset{\sim}{C}$. Orthogonal matrices are used frequently in statistics, especially in linear models and multivariate analysis (see, for example, Graybill, 1961, Chap. 11; Searle, 1971, Chap. 2; Anderson, 1965; and James, 1954).

Orthogonal matrices of determinant 1 represent elements of the rotation group in n dimensions. Gel'fand et al. (1963) and Murnaghan (1938) give extensive discussions of the representation of the n-dimensional rotation group. Hoffman et al. (1972) and Raffenetti and Ruedenberg (1970) represented the class of n-dimensional orthogonal matrices in terms of generalized Eulerian angles. The

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representation of three-dimensional orthogonal matrices by Eulerian angles has long been used in the study of the motion of a rigid body (Euler, 1776, Whittaker, 1927, pp. 9-10). For further ideas and a three-dimensional application, see Moran (1975).

The n^2 elements of an orthogonal matrix are subject to $\frac{1}{2}n(n+1)$ constraints. It is therefore not surprising that they can be represented by only $n^2 - \frac{1}{2}n(n+1) = \frac{1}{2}n(n-1)$ independent parameters. A representation is convenient if the whole of a matrix can be quickly computed from the $\frac{1}{2}n(n-1)$ parameters. Such a representation facilitates the search for an orthogonal matrix that satisfies some optimality criterion. The independent parameters can be used also in integrating a function over the n-dimensional orthogonal group (Murnaghan, 1938, pp. 230-242), which is defined as the set of all $n \times n$ orthogonal matrices with the operation of matrix multiplication.

As far as we know, the various methods of parameterizing orthogonal matrices are not available in the statistical literature. Our aim is to bring several of these methods to the attention of the statistical profession, and we do not claim mathematical originality, although probably a few of our comments have some novelty.

First we mention some applications. The cited references may be consulted for more details. The rotation group of $n \times n$ orthogonal matrices will be denoted by $O(n)$.

2. Some Applications in Statistics of Parameterization of the Orthogonal Group.

(a) A parameterization of $O(n)$ can be used to define an invariant (Haar) measure, μ, on $O(n)$. This measure is invariant in the sense that if a set G of orthogonal n by n matrices has measure $\mu(G)$ then, for every orthogonal n by n matrix $\underset{\sim}{C}$, $\mu(G) = \mu(G\underset{\sim}{C}) = \mu(\underset{\sim}{C}G)$ and $G\underset{\sim}{C}$ [and $\underset{\sim}{C}G$] denotes the set of matrices obtained by multiplying all the matrices in G on the right [left] by $\underset{\sim}{C}$. Haar measure is unique up to a positive multiplicative constant. In accordance, for example, with James (1954, p. 53), the Haar measure $\mu(G)$, if it exists, is given by the $\frac{1}{2}n(n-1)$-fold integral

$$\mu(G) = \int_G \prod_{i,j}^{1<i<j<n} (\underset{\sim}{c}_i' \cdot d\underset{\sim}{c}_j) , \quad G \subset O(n)$$

where $\underset{\sim}{c}_i$ and $\underset{\sim}{c}_j$ are the i^{th} and j^{th} column vectors of an orthogonal matrix $\underset{\sim}{C}$, $(\underset{\sim}{c}_i' \cdot d\underset{\sim}{c}_j)$ denotes a scalar product, and the product of differential forms is to be interpreted as an exterior product. (Exterior products are explained, for example, by James, 1954, p. 46.) For example, if $n = 2$, the differential form, $\Pi(\underset{\sim}{c}_i' \cdot d\underset{\sim}{c}_j)$, for

$$\underset{\sim}{C} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} , \quad 0 \leq \theta < 2\pi ,$$

is $(\underset{\sim}{c}_1' \cdot d\underset{\sim}{c}_2) = d\theta$.

The Haar measure has been used to derive the distribution of the canonical correlation coefficients (James, 1954). Anderson (1965) used the representation given by formula (3.2) of Section 3 below to obtain the joint distribution of the eigenvalues of the sample variance-covariance matrix. See also, for example, Wijsman (1957), Chattopadhyay et al. (1976).

(b) When carrying out simulation experiments in regression theory, the condition number of $\underset{\sim}{X}'\underset{\sim}{X}$ is of interest, where $\underset{\sim}{X}$ is the matrix associated with the regression model. This condition number is defined (Hartree, 1955, p. 153) as the ratio of the largest to the smallest of the eigenvalues of $\underset{\sim}{X}'\underset{\sim}{X}$. George Terrell pointed out (private communication) that by applying random orthogonal transformations to $\underset{\sim}{X}$, we can generate several different $\underset{\sim}{X}$ matrices for which the condition numbers are all equal. This would be convenient in the simulation experiments. The generation of such random orthogonal transformations can be facilitated by utilizing the independent parameters obtained through parameterization of the orthogonal matrices representing these transformations.

(c) The simultaneous diagonalization of several matrices is of considerable interest in statistics, especially in the analysis of random - or mixed-effects models. Let $\underset{\sim}{A}_1, \underset{\sim}{A}_2, \ldots, \underset{\sim}{A}_\ell$ be ℓ (≥ 2) positive definite symmetric matrices of order $p \times p$. Suppose that these matrices are not simultaneously diagonalizable (because they do not commute), and we wish to find an orthogonal matrix, $\underset{\sim}{B}$, which makes them simultaneously "as diagonal as possible". Flury and Gautschi (1986, p. 170) introduced a measure of simultaneous deviation of the matrices, $\underset{\sim}{B}\underset{\sim}{A}_1\underset{\sim}{B}'$, $\underset{\sim}{B}\underset{\sim}{A}_2\underset{\sim}{B}'$, ..., $\underset{\sim}{B}\underset{\sim}{A}_\ell\underset{\sim}{B}'$, from diagonality. This measure is given by the function

$$\chi(\underset{\sim}{B}, \underset{\sim}{A}_1, \underset{\sim}{A}_2, \ldots, \underset{\sim}{A}_\ell; n_1, n_2, \ldots, n_\ell) =$$

$$\prod_{i=1}^{\ell} \{|\operatorname{diag}(\underset{\sim}{B}\underset{\sim}{A}_i\underset{\sim}{B}')|/|\underset{\sim}{B}\underset{\sim}{A}_i\underset{\sim}{B}'|\}^{n_i} , \tag{2.1}$$

where $\operatorname{diag}(\underset{\sim}{B}\underset{\sim}{A}_i\underset{\sim}{B}')$ is a diagonal matrix having the same diagonal elements as $\underset{\sim}{B}\underset{\sim}{A}_i\underset{\sim}{B}'$ ($i = 1, 2, \ldots, \ell$), $|\cdot|$ denotes the determinant of a matrix, and $n_1, n_2, \ldots, n_\ell$ are positive weights. It is known that $\chi \geq 1$ with equality occurring if and only if $\underset{\sim}{B}$ diagonalizes the $\underset{\sim}{A}_i$'s. It is therefore of interest to find the minimum of χ over the rotation group $O(p)$.

The determination of the optimal orthogonal matrix, $\underset{\sim}{B}_0$, that minimizes χ in (2.1) can be reduced to an optimization problem in $\frac{1}{2}p(p-1)$ dimensions since this is the number of independent parameters that represent the elements of $O(P)$. Flury and Gautschi (1986) did not follow this procedure; instead, they introduced an iterative algorithm whereby a converging sequence of orthogonal matrices, $\underset{\sim}{B}^{(0)}$, $\underset{\sim}{B}^{(1)}$, ... , was derived such that $\chi(\underset{\sim}{B}^{(j+1)}) \leq \chi(\underset{\sim}{B}^{(j)})$, $j = 0, 1, 2, \ldots$. All pairs of columns of the orthogonal matrix $\underset{\sim}{B}^{(j)}$ obtained in the j^{th} iteration ($j = 0, 1, 2, \ldots$) are subjected to rotations by a specific 2×2 orthogonal matrix parameterized by a single parameter. This yields the matrix $\underset{\sim}{B}^{(j+1)}$ and the process is repeated until some convergence criterion is met.

(d) The need for parameterization arises in response surface analysis. Consider a linear model of the form

$$\underset{\sim}{Y} = \underset{\sim}{X}\underset{\sim}{\beta} + \underset{\sim}{\epsilon}, \tag{2.2}$$

where $\underset{\sim}{Y}$ is the vector of observations, $\underset{\sim}{\beta}$ is a vector of unknown parameters, and $\underset{\sim}{X}$ is a known matrix of order $n \times p$ and rank p. The elements of $\underset{\sim}{X}$ are functions of the settings of m input variables denoted by $x_1, x_2, \ldots, x_m$. The $n \times m$ matrix, $\underset{\sim}{D} = (x_{ui})$, where x_{ui} is the setting of the i^{th} variable at the u^{th} experimental run ($u = 1, 2, \ldots, n$; $j = 1, 2, \ldots, m$), is called the design matrix. The elements of the error vector $\underset{\sim}{\epsilon}$ in (2.2) are assumed to be independently and identically distributed random variables with zero means and variances equal to σ^2.

Tests of significance concerning the parameter vector $\underset{\sim}{\beta}$ in (2.2) depend on the assumption that $\underset{\sim}{\epsilon}$ is normally distributed. The effect of nonnormality of the error distribution on these tests has been studied by several authors (see, for example, Pearson, 1931; Geary, 1947; Gayen, 1950; and David and Johnson, 1951a, 1951b). Box and Watson (1962) pointed out that the sensitivity to nonnormality depends very much on the settings of the input variables specified in the design matrix. This was also demonstrated by Vuchkov and Solakov (1980).

Thus, a properly chosen design matrix can lead to tests that are resistant, or robust, to failure of the normality assumption.

Box and Watson (1962) introduced a design robustness criterion for a model of the form (2.2) of degree one (a first-order model), which can be rewritten as

$$\underset{\sim}{Y} = \underset{\sim}{1}\beta_0 + \underset{\sim}{D}\tau + \underset{\sim}{\epsilon} \,, \tag{2.3}$$

where $\underset{\sim}{1}$ is a column vector of ones of order $n \times 1$, $\underset{\sim}{D}$ is the design matrix such that $\underset{\sim}{X} = [\underset{\sim}{1} : \underset{\sim}{D}]$, and $(\beta_0, \tau')' = \underset{\sim}{\beta}$. Box and Watson's criterion is for testing the hypothesis

$$H_0\colon \underset{\sim}{\tau} = \underset{\sim}{0} \tag{2.4}$$

using the mean square ratio

$$F(\underset{\sim}{D}) = [\underset{\sim}{y}'\underset{\sim}{D}(\underset{\sim}{D}'\underset{\sim}{D})^{-1}\underset{\sim}{D}'\underset{\sim}{y}/m]/[\underset{\sim}{y}'(\underset{\sim}{I} - \underset{\sim}{X}(\underset{\sim}{X}'\underset{\sim}{X})^{-1}\underset{\sim}{X}')\underset{\sim}{y}/(n-m-1)] \,.$$

They showed that in nonnormal situations, $F(\underset{\sim}{D})$ is distributed approximately under H_0 as an F-distribution with modified degrees of freedom given by $\nu_1 = \eta m$ and $\nu_2 = \eta(n-m-1)$. Here the corrective factor η is equal to unity if $g(\underset{\sim}{D}) = 0$ regardless of the y's or their distribution, where

$$g(\underset{\sim}{D}) = d - m(m+2)(n-1)/[n(n+1)] \,, \tag{2.5}$$

and $d = \sum_{i=1}^{m} d_{ii}^2$ with d_{ii} being the i^{th} diagonal element of $\underset{\sim}{D}(\underset{\sim}{D}'\underset{\sim}{D})^{-1}\underset{\sim}{D}'$. Since η is equal to unity when the error distribution is normal, a design matrix satisfying

$$g(\underset{\sim}{D}) = 0 \tag{2.6}$$

will result in an approximate F statistic with degrees of freedom identical to those obtained under normality. Consequently, the design matrix can determine whether the distribution of $F(\underset{\sim}{D})$ is insensitive (robust) to nonnormality. The matrix $\underset{\sim}{D}(\underset{\sim}{D}'\underset{\sim}{D})^{-1}\underset{\sim}{D}'$, being idempotent, can be expressed in the form

$$\underset{\sim}{D}(\underset{\sim}{D}'\underset{\sim}{D})^{-1}\underset{\sim}{D}' = \underset{\sim}{P}\,\mathrm{diag}(\underset{\sim}{I}_m, \underset{\sim}{0})\underset{\sim}{P}' ,$$

where $\underset{\sim}{P}$ is an orthogonal matrix. In this way, the parameterization of $\underset{\sim}{D}(\underset{\sim}{D}'\underset{\sim}{D})^{-1}\underset{\sim}{D}'$ can be reduced to that of an orthogonal matrix. The quantity, d, in (2.5) can be regarded as a function, $h(\underset{\sim}{P})$, of $\underset{\sim}{P}$ and (2.5) becomes

$$g(\underset{\sim}{D}) = h(\underset{\sim}{P}) - m(m+2)(n-1)/[n(n+1)] . \qquad (2.7)$$

For a fixed n, one method to implement the Box-Watson criterion is to find $\underset{\sim}{P}$ so that $g^2(\underset{\sim}{D})$ has an absolute minimum over the rotation group $O(n)$. If this absolute minimum is zero, then the Box-Watson criterion is satisfied. Otherwise, the optimal design that minimizes $g^2(\underset{\sim}{D})$ is the design that comes "closest" to satisfying this criterion. For more details concerning this matter see Khuri and Myers (1981).

The minimization process can be carried out by expressing $h(\underset{\sim}{P})$ in (2.7) in terms of the parameters of the orthogonal matrix $\underset{\sim}{P}$.

We now describe various methods of parameterization.

3. How to Parameterize an Orthogonal Matrix.

The four methods we shall discuss are (i) expressing an orthogonal matrix in the form $e^{\underset{\sim}{T}}$ where $\underset{\sim}{T}$ is skew-symmetric, (ii) using Cayley's transformation which also gives an expression in terms of a skew-symmetric matrix, (iii) using Eulerian angles for the three-dimensional case, and (iv) using generalized Eulerian angles for the n-dimensional case.

(i) If $\underset{\sim}{Q}$ is an $n \times n$ orthogonal matrix with determinant 1, then it can be written in the form

$$\mathbf{Q} = e^{\mathbf{T}} , \tag{3.1}$$

where $\mathbf{T}$ is a skew-symmetric matrix (see, for example, Gantmacher, 1959, p. 288). (The exponential is of course definable as an infinite series.) The elements of $\mathbf{T}$, above its main diagonal, can be used to parameterize $\mathbf{Q}$.

Now, if $\mathbf{Q}$ is given, then to find $\mathbf{T}$ we can first find the eigenvalues of $\mathbf{Q}$. These are necessarily of the form $e^{\pm i\phi_1}, e^{\pm i\phi_2}, \ldots , e^{\pm i\phi_q}, 1$, where the eigenvalue 1 is of multiplicity $(n - 2q)$, and none of the real numbers ϕ_j ϕ_j is a multiple of 2π $(j = 1, 2, \ldots , q)$. (Those that are odd multiples of π give an even number of eigenvalues equal to -1.) If we denote the matrix $\begin{bmatrix} a & b \\ -b & a \end{bmatrix}$ by $[a + bi]$, a notation that is reasonable because the 2×2 matrices form a representation of complex numbers, then $\mathbf{Q}$ can be written (Gantmacher, 1959, p. 288), as the product of three <u>real</u> matrices,

$$\mathbf{Q} = \mathbf{Q}_1 \operatorname{diag}([e^{i\phi_1}], \ldots , [e^{i\phi_q}], 1, \ldots , 1)\mathbf{Q}_1' . \tag{3.2}$$

Here $\mathbf{Q}_1$ is an orthogonal matrix of the form

$$\mathbf{Q}_1 = [\mathbf{x}_1, \mathbf{y}_1, \mathbf{x}_2, \mathbf{y}_2, \cdots , \mathbf{x}_q, \mathbf{y}_q, \mathbf{x}_{2q+1}, \cdots , \mathbf{x}_n]$$

such that $\mathbf{x}_j + i\mathbf{y}_j$ is an eigenvector with eigenvalue $e^{i\phi_j}$ $(j = 1, \ldots , q)$, and $\mathbf{x}_k$ is an eigenvector with eigenvalue 1 $(k = 2q + 1, \ldots , n)$.

We now define the skew-symmetric matrix $\mathbf{T}$ by the equation

$$\mathbf{T} = \mathbf{Q}_1 \operatorname{diag}([i\phi_1], \ldots , [i\phi_q], 0, \ldots , 0)\mathbf{Q}_1' . \tag{3.3}$$

Since $e^{[i\phi_j]} = [e^{i\phi_j}]$ we have $\mathbf{Q} = e^{\mathbf{T}}$ as required.

We note that

$$\underset{\sim}{Q} = \prod_{j=0}^{q-1} \underset{\sim}{R}_j$$

where

$$\underset{\sim}{R}_j = \underset{\sim}{Q}_1 \operatorname{diag}(\underset{\sim}{I}_{2j}, [e^{i\phi_{j+1}}], \underset{\sim}{I}_{n-2j-2})\underset{\sim}{Q}_1' , \quad j = 0, \ldots , q-1 ,$$

and where $\underset{\sim}{I}_{2j}$ and $\underset{\sim}{I}_{n-2j-2}$ are the identity matrices of dimensions 2j and n-2j-2, respectively. If Π_{j+1} is a plane parallel to both the vectors $\underset{\sim}{x}_{j+1}$ and $\underset{\sim}{y}_{j+1}$, then $\underset{\sim}{R}_j$ represents a rotation of the n-space leaving fixed every point in the (n-2)-space orthogonal to Π_{j+1} (Vitali, 1928). Thus $\underset{\sim}{Q}$ represents the product of q such simple rotations. When n = 3 and q = 1, this is a familiar fact in dynamics, known to Euler. To obtain a power $\underset{\sim}{Q}^{\alpha}$ we could multiply all the angles of rotation by α.

We note also that

$$\begin{aligned} \underset{\sim}{T}(\underset{\sim}{x}_j + i\underset{\sim}{y}_j) &= i\phi_j(\underset{\sim}{x}_j + i\underset{\sim}{y}_j) , \quad j = 1, 2, \ldots , q , \\ \underset{\sim}{T}\underset{\sim}{x}_k &= 0 \qquad\qquad\qquad\quad , \quad k = 2q+1, \ldots , n . \end{aligned} \tag{3.4}$$

Equations (3.4) state that $\underset{\sim}{x}_j + i\underset{\sim}{y}_j$ is an eigenvector of $\underset{\sim}{T}$ with eigenvalue $i\phi_j$, and that $\underset{\sim}{x}_k$ is an eigenvector of $\underset{\sim}{T}$ with zero eigenvalue. Since the eigenvalues of $\underset{\sim}{T}$ are purely imaginary or zero (at least one of them is zero if n is odd), and the imaginary ones pair off in conjugate pairs $\pm i\phi_1, \ldots , \pm i\phi_q$, it follows that (3.3) gives a representation of a real skew-symmetric matrix in terms of its eigenvalues and eigenvectors (Gantmacher, 1959, p. 285). This observation enables us to calculate $\underset{\sim}{Q}$ if $\underset{\sim}{T}$ is given and if (3.1) is known to be true. We first put $\underset{\sim}{T}$ in the form (3.3), then we calculate $\underset{\sim}{Q}$ by (3.2). For convenience in computing the eigenvalues and eigenvectors of $\underset{\sim}{T}$, we note that $\underset{\sim}{x}_j$ and $\underset{\sim}{y}_j$ $(j = 1, \ldots, q)$ are eigenvectors of the symmetric matrix $\underset{\sim}{T}^2$ with eigenvalue $-\phi_j^2$. This can be easily seen from (3.3), which when both sides are squared gives

$$\underset{\sim}{T}^2 = -\sum_{j=1}^{q} \phi_j^2(\underset{\sim}{x}_j\underset{\sim}{x}_j' + \underset{\sim}{y}_j\underset{\sim}{y}_j') .$$

<u>Example, n = 3</u>. In three dimensions any orthogonal matrix $\underset{\sim}{Q}$, with determinant 1, has the form

$$\underset{\sim}{Q} = \exp\begin{bmatrix} 0 & c & -b \\ -c & 0 & a \\ b & -a & 0 \end{bmatrix} .$$

The eigenvalues of

$$\underset{\sim}{T} = \begin{bmatrix} 0 & c & -b \\ -c & 0 & a \\ b & -a & 0 \end{bmatrix}$$

are $i\rho$, $-i\rho$, and 0, where $\rho = (a^2 + b^2 + c^2)^{\frac{1}{2}}$. The normalized eigenvector with eigenvalue 0 is $\underset{\sim}{w} = \rho^{-1}[a, b, c]'$ and the other normalized eigenvectors can be chosen as $\underset{\sim}{u} \pm i\underset{\sim}{v}$ where

$$\underset{\sim}{u} = (b^2 + c^2)^{-\frac{1}{2}}[0, c, -b]'$$

and

$$\underset{\sim}{v} = \rho^{-1}(b^2 + c^2)^{-\frac{1}{2}}[b^2 + c^2, -ab, -ac]' .$$

The vectors $\underset{\sim}{u}$ and $\underset{\sim}{v}$ are orthonormal eigenvectors of $\underset{\sim}{T}^2$ with the eigenvalue

$-\rho^2$.

From (3.2), we have

$$\underset{\sim}{Q} = [\underset{\sim}{u}, \underset{\sim}{v}, \underset{\sim}{w}]\mathrm{diag}\{[e^{-i\rho}],1\}[\underset{\sim}{u}, \underset{\sim}{v}, \underset{\sim}{w}]' \; .$$

The matrix $\underset{\sim}{Q}$ represents a rotation of the 3-space about a line whose direction cosines are $(a/\rho, b/\rho, c/\rho)$.

(ii) If $\underset{\sim}{Q}$ is an orthogonal matrix that does not have the eigenvalue -1, then it may be written in Cayley's form (Gantmacher, 1959, p. 289).

$$\underset{\sim}{Q} = (\underset{\sim}{I} - \underset{\sim}{S})(\underset{\sim}{I} + \underset{\sim}{S})^{-1} \tag{3.5}$$

where $\underset{\sim}{S}$ is a skew-symmetric matrix. [$\underset{\sim}{I} + \underset{\sim}{S}$ is never singular if $\underset{\sim}{S}$ is skew-symmetric. A proof of this fact is given by Ferrar (1950, p. 163) who attributes the fact to Cayley. A simpler proof is that all the eigenvalues of a skew-symmetric matrix $\underset{\sim}{S}$ are purely imaginary or zero (because it is Hermitian) and therefore -1 cannot be an eigenvalue of $\underset{\sim}{S}$.] The form (3.5) has the advantage of defining $\underset{\sim}{Q}$ as a one-to-one function of $\underset{\sim}{S}$, but it has the disadvantage of being restricted to those orthogonal matrices that do not have the eigenvalue -1. If this condition is not assumed, $\underset{\sim}{Q}$ can still be written in the form (Ferrar, 1950, p. 164)

$$\underset{\sim}{Q} = \underset{\sim}{J}(\underset{\sim}{I} - \underset{\sim}{S})(\underset{\sim}{I} + \underset{\sim}{S})^{-1} \tag{3.6}$$

where $\underset{\sim}{J}$ is a diagonal matrix in which each element on the diagonal is either 1 or -1 (and where $\underset{\sim}{S}$ is skew-symmetric). This representation can be made unique by insisting that all the plus 1's precede all the minus 1's along the diagonal of $\underset{\sim}{J}$. When this representation is used we must supplement the $\frac{1}{2}n(n-1)$ parameters in $\underset{\sim}{S}$ with an assumption for the number, r, of plus 1's in $\underset{\sim}{J}$.

(iii) In three dimensions orthogonal transformations with determinant 1 are of course represented by the rotation of a rigid body free to turn about a point O. The motion of this body is determined by three independent angles known as Eulerian angles (Euler, 1776; Whittaker, 1927, p. 9; Condon, 1958, p. 6). These angles can be introduced in various ways. The following one is used by Condon:

Let OXYZ be a right-handed system of rectangular axes fixed in space. Let Oxyz be rectangular axes fixed relatively to the body and moving with it, such that before the displacement the two sets of axes OXYZ and Oxyz are coincident in position. Let $\underset{\sim}{v}_Z$ and $\underset{\sim}{v}_z$ be unit vectors in the positive directions of the Z and z axes, respectively, and let $\underset{\sim}{K} = \underset{\sim}{v}_Z \times \underset{\sim}{v}_z$ be their vector product. Denote the angles ZOz, XOK, KOx by θ, ϕ, ψ, respectively. These are the three Eulerian angles.

By a remark made in Section 3(i) the total movement of the body is equivalent to a rotation. This rotation is represented by the product of three matrices, thus:

$$\underset{\sim}{Q} = \mathrm{diag}([e^{i\psi}], 1)\mathrm{diag}(1, [e^{i\theta}])\mathrm{diag}([e^{i\phi}], 1)$$

$$= \begin{bmatrix} \cos\phi\cos\psi - \sin\phi\cos\theta\sin\psi & \sin\phi\cos\psi + \cos\phi\cos\theta\sin\psi & \sin\theta\sin\psi \\ -\cos\phi\sin\psi - \sin\phi\cos\theta\cos\psi & -\sin\phi\sin\psi + \cos\phi\cos\theta\cos\psi & \sin\theta\cos\psi \\ \sin\phi\sin\theta & -\cos\phi\sin\theta & \cos\theta \end{bmatrix} \tag{3.7}$$

This then provides a parameterization in three dimensions. The parameterization is unique if, for example, $0 \leqslant \theta < 2\pi$, $0 \leqslant \phi < 2\pi$, and $0 \leqslant \psi \leqslant \pi$.

(iv) A generalization of the concept of the three-dimensional Eulerian angles to n dimensions was given by Raffenetti and Ruedenberg (1970). Formulae and a computer program were derived that expressed an arbitrary orthogonal matrix of order $n \times n$ in terms of $\frac{1}{2}n(n-1)$ angular variables. A general n-dimensional orthogonal matrix, $\underset{\sim}{Q}$, can be constructed by the sequence of recurrence relations

$$
\begin{aligned}
&\underset{\sim}{Q}^{(1)} = \pm 1 \\
&\underset{\sim}{q}^{(i)} = \operatorname{diag}(\underset{\sim}{Q}^{(i-1)}, 1), && i = 2, 3, \ldots, n, \\
&\underset{\sim}{A}^{(i)} = a_{i-1,i}a_{i-2,i} \cdots a_{1,i}, && i = 2, 3, \ldots, n, \\
&\underset{\sim}{Q}^{(i)} = \underset{\sim}{A}^{(i)} \underset{\sim}{q}^{(i)}, && i = 2, 3, \ldots, n, \\
&\underset{\sim}{Q} = \underset{\sim}{Q}^{(n)}
\end{aligned}
$$

where $(a_{i,j})$ $(i = 1, 2, \ldots, n;\ j = 1, 2, \ldots, n;\ i < j)$ is an $n \times n$ matrix whose diagonal elements are 1 except for the diagonal elements in the i^{th} and j^{th} columns, which are $\cos\gamma_{ij}$; all off-diagonal elements are 0 except for the one corresponding to the intersection of the i^{th} row and the j^{th} column, which is $\sin\gamma_{ij}$, and that on the intersection of the j^{th} row and the i^{th} columns which is $-\sin\gamma_{ij}$. The choice $\underset{\sim}{Q}^{(1)} = 1$ yields an orthogonal matrix $\underset{\sim}{Q} = \{Q_{ij}\}$ with determinant 1, and the choice $\underset{\sim}{Q}^{(1)} = -1$ yields a matrix $\underset{\sim}{Q}$ with determinant -1.

Conversely, if an orthogonal matrix, $\underset{\sim}{U} = \{U_{ij}\}$, is given, then the corresponding angular variables are found by minimizing the function $f(\gamma)$ $= \sum_{i,j} [U_{ij} - Q_{ij}(\underset{\sim}{\gamma})]^2$, and where $\underset{\sim}{\gamma} = (\gamma_{12}, \gamma_{13}, \ldots, \gamma_{n-1,n})'$ $(i, j = 1, 2, \ldots, n)$, and the elements of $\underset{\sim}{Q}$ are found by a prescribed recurrence scheme. Hoffman et al (1972), however, give algebraic inversion formulae, and a computer program, for the angular variables in terms of the elements of the orthogonal matrix.

4. A Problem Concerning Haar Measure.

It would be of value for numerical integration over the orthogonal group if Haar measure could be generated by $\frac{1}{2}n(n-1)$ statistically independent random angles each uniformly distributed. For we could then approximate the integration over the orthogonal group by a discrete sum over points uniformly spaced on circles. In three dimensions the Eulerian angles do not serve this purpose. For suppose that ϕ, θ, and ψ are each uniformly distributed. Then $\cos\theta$ cannot have the same distribution as the other elements on the diagonal of the matrix in (3.7), so that the transformation is not symmetrical with respect to the axes. Thus the distribution cannot be invariant under all rotations.

One can arrive at Haar measure for the three-dimensional rotation group by choosing an axis of rotation with uniform polar angles in $(0, \pi)$ and $(0, 2\pi)$ and then choosing an angle ω of rotation with uniform distribution in $(0, 2\pi)$. The matrix giving this orthogonal transformation, expressed in terms of ω and the direction cosines, $\cos\lambda$, $\cos\mu$, and $\cos\nu$, of the axis of rotation, is

$$\begin{bmatrix} 1 - 2s_1^2h^2 & 2c_1c_2h^2 - c_3s & 2c_1c_3h^2 + c_2s \\ 2c_1c_2h^2 + c_3s & 1 - 2s_2^2h^2 & 2c_2c_3h^2 - c_1s \\ 2c_1c_3h^2 - c_2s & 2c_2c_3h^2 + c_1s & 1 - 2s_3^2h^2 \end{bmatrix}, \qquad (4.1)$$

where $s = \sin\omega$, $h = \sin\frac{1}{2}\omega$, $s_1 = \sin\lambda$, $s_2 = \sin\mu$, $s_3 = \sin\nu$, $c_1 = \cos\lambda$, $c_2 = \cos\mu$, $c_3 = \cos\nu$. This result can be readily derived from Whittaker (1927, p. 8). Formula (4.1) provides a matrix representation of the rotation group and it is equipped with Haar measure if λ, μ, ν and ω have uniform distributions in $(0, 2\pi)$, $(0, 2\pi)$, $(0, 2\pi)$, and $(0, \pi)$ respectively. It seems to be difficult to generalize this result to n dimensions.

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